Additive Invariants of Open Petri Nets

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In this talk, we will classify all N-valued invariants of open Petri nets which are additive with respect to composition and monoidal product in the category of open Petri nets, **OPetri**. Formally, these invariants are monoidal functors **OPetri** \rightarrow **B**N. The additive invariants of open Petri nets are completely determined by their values on a particular class of single-transition Petri nets. For open Petri nets whose legs are monic maps, the additive invariants are determined by their values on all single-transition Petri nets as well as transitionless Petri nets. Our results confirm a conjecture made by John Baez during the AMS 2022 Mathematical Research Communities workshop. The paper-length version is available at https://arxiv.org/abs/2303.01643.

1 MOTIVATION

Petri nets represent many kinds of processes (concurrent, asynchronous, distributed, parallel, nondeterministic, and stochastic, to name a few) in which some entities (the species) undergo transformations (transitions) in order to be converted into other kinds of entities [1, 6, 7, 9, 10, 13, 15, 20]. For example, in chemistry, there are vast databases recording many kinds of chemical reactions and their associated Petri nets [8, 12, 16, 19] which are studied empirically by computationally seeking patterns, *motifs* [18], and *numerical invariants* that arise within this data. For instance, these invariants may include calculating the production of iron or the appearances of a catalyst in a reaction.

Often due to the sheer size of the Petri nets in such databases, it is convenient to consider a large Petri net as built out of smaller constituent nets which are "glued" together to form the whole. The compositional structure of Petri nets can be leveraged in studying invariants of Petri nets so long as the invariants behave nicely with respect to this kind of gluing. An example of such "nice" behaviour is additivity: if *P* is the composite of Petri nets P_1, \ldots, P_n , then the value of an additive invariant on *P* reduces to computing the invariant on each of P_1, \ldots, P_n and summing the results.

Additive invariants are examples of compositional semantics for Petri nets. Their relative simplicity compared with the semantics of mass action kinetics — a natural number rather than a differential equation — is practical for developing domain specific Petri nets. For example, an invariant can express a constraint imposed by domain experts or discovered empirically by analyzing real-world Petri nets. The compositional nature of such invariants is useful for constraint verification and modularly building networks to satisfy a certain constraint. These features can be implemented straightforwardly in the software package AlgebraicPetri.jl.

The classification of these additive invariants relies on two decomposition lemmas for open Petri nets. Given the large literature on open Petri nets in applied category theory, these lemmas are of independent significance.

Composition of open Petri nets has a rich history in applied category theory [2, 3, 17], and the decomposition of graphical models has been previously studied. Nielsen et. al. [14] prove that a finite Petri net can be built from single-place and single-transition Petri nets via a collection of many operations on nets known as *combinators*. Gadduci and Heckel [5] present a kindred theorem for the decomposition of graphs into atomic components.

2 CLASSIFYING ADDITIVE INVARIANTS

The category **OPetri** is a decorated cospan category [4] whose objects are finite sets and whose morphisms are cospans of finite sets where the apex is the species set of a Petri net [2]. An **additive invariant** of open Petri nets is a monoidal functor $F: \text{$ **OPetri** $} \rightarrow \mathbf{BN}$ where \mathbf{BN} is the one-object category induced by the monoid $(\mathbb{N}, +)$. The monoidal product of \mathbf{BN} is also given by +. Note that the literature on Petri nets uses the word "invariant" for a different concept, namely a solution to the equation Ax = 0 or $A^Ty = 0$ where A is the Petri net's incidence matrix [11]. Whereas those invariants are quantities that take the same value for all markings reachable within a Petri net, the invariants presented in this abstract are quantities assigned to a Petri net that respect composition.

An additive invariant depends solely on the number of input arcs and output arcs of each transition. We define canonical open Petri nets with *m* input arcs and *n* output arcs as follows: Let $P_{m,n}$ be the Petri net with a single transition that has *m* distinct input species and *n* distinct output species. Let $\mathcal{P}_{m,n}$ be the open Petri net decorated by $P_{m,n}$ and whose underlying cospan is the identity. The additive invariants of open Petri nets are completely determined by their behavior on the open Petri nets of the form $\mathcal{P}_{m,n}$. This idea is formalized in the following theorem.

THEOREM 2.1. For any two $m, n \in \mathbb{N}$, there is a functor

$F_{m,n}: \text{ OPetri} \rightarrow \mathbb{BN}$

which maps each open Petri net to the total number of transitions with exactly m input arcs and n output arcs. Furthermore, any additive invariant $G: \text{OPetri} \rightarrow \mathbb{BN}$ is completely determined — as a linear combination of the functors $F_{m,n}$ defined above — by its values on the family $\mathcal{P}_{m,n}$. In particular, we have

$$G(-) = \sum_{m,n \in \mathbb{N}} G(\mathcal{P}_{m,n}) F_{m,n}(-)$$



Figure 1: An open Petri net with three transitions. The transitions labeled α and γ both have one input arc and two output arcs and so $F_{1,2}$ applied to this open Petri net is 2. Conversely, the transition labeled β has one input arc and one output arc. Therefore, $F_{1,1}$ applied to this open Petri net is 1.

We are also interested in the category of **mope nets**, open Petri nets whose legs are monomorphisms. These Petri nets form a category **MOPetri** which is a wide subcategory of **OPetri**. In **OPetri**, composing open Petri nets can identify two species in the decoration of one of the factors. For example, an input species and an output species of a transition may be identified so that they appear as a single catalyst in the composite. This identification is not possible in **MOPetri**. Instead, composition in **MOPetri** preserves the relation between each transition and its input and output species.

Whereas the additive invariants of open Petri nets depend on their behavior on the open Petri nets $\mathcal{P}_{m,n}$, we prove that the additive invariants of mope nets depend on their behavior on the following two classes of mope nets:

- **Boundary nets**, which are transitionless open Petri nets whose underlying cospan is either of the form $0 \rightarrow S \xleftarrow{}^{1_S} S$ or $S \xrightarrow{}^{1_S} S \leftarrow 0$.
- **Body nets**, which are open Petri nets whose underlying cospan is the identity and whose decoration has a single transition.

Finer additive invariants of mope nets exist, because the identity of species is preserved by composition in **MOPetri**.

For example, counting catalysts - species which are both consumed and emitted by a transition - is an additive invariant of mope nets.

3 DECOMPOSITION OF OPEN PETRI NETS

The proofs of the classification theorems rely on two decomposition lemmas. The decomposition lemmas are of independent interest, because they allow us to study open Petri nets as compositions of factors with one or zero transitions.

The first decomposition lemma specifies that an open Petri net can be decomposed into the composite and monoidal product of transitionless open Petri nets and open Petri nets of the form $\mathcal{P}_{m,n}$. This lemma is used to prove Theorem 2.1, and Figure 2 gives an application of it.

The second decomposition lemma specifies that an open Petri net can be decomposed into the composite of transitionless open Petri nets and body nets. This lemma is used to prove the analogous classification theorem for mope nets.



Figure 2: The decomposition of the open Petri net depicted in Figure 1 as defined in the first decomposition lemma. The decomposition is Q; $(\mathcal{G}_0 \oplus \mathcal{G}_1 \oplus \mathcal{G}_2 \oplus \mathcal{G}_3)$; Q'. Graphically each \mathcal{G}_i is enclosed by a grey box and they are shown in numerical order from top to bottom.

REFERENCES

- J. C. Baez and J. D. Biamonte. *Quantum Techniques in Stochastic Mechanics*. World Scientific, 2018. URL: https://doi.org/10.48550/arXiv. 1209.3632.
- [2] J. C. Baez and B. S. Pollard. A Compositional Framework for Reaction Networks. *Reviews in Mathematical Physics*, 29(09):1750028, 2017. URL: https://doi.org/10.1142/S0129055X17500283.

- [3] Paolo Baldan, Andrea Corradini, Hartmut Ehrig, and Reiko Heckel. Compositional modeling of reactive systems using open nets. In CON-CUR 2001–Concurrency Theory: 12th International Conference Aalborg, Denmark, August 20–25, 2001 Proceedings 12, pages 502–518. Springer, 2001.
- [4] B. Fong. The Algebra of Open and Interconnected Systems. Ph.D. thesis, Computer Science Department, University of Oxford.
- [5] Fabio Gadducci and Reiko Heckel. An inductive view of graph transformation. In *International Workshop on Algebraic Development Techniques*, pages 223–237. Springer, 1997.
- [6] P. J. Haas. Stochastic Petri Nets: Modelling, Stability, Simulation. Springer New York, NY, 2002. URL: https://doi.org/10.1007/b97265.
- [7] K. Jensen and L. M. Kristensen. Coloured Petri Nets: Modelling and Validation of Concurrent Systems. Springer Science & Business Media, 2009.
- [8] G. M. Keserű, T. Soós, and C. O. Kappe. Anthropogenic Reaction Parameters–The Missing Link Between Chemical Intuition and the Available Chemical Space. *Chemical Society Reviews*, 43(15):5387–5399, 2014. URL: https://doi.org/10.1039/C3CS60423C.
- I. Koch. Petri Nets-A Mathematical Formalism to Analyze Chemical Reaction Networks. *Molecular Informatics*, 29(12):838–843, 2010. URL: https://doi.org/10.1002/minf.201000086.
- [10] I. Koch, W. Reisig, and F. Schreiber. Modeling in Systems Biology: the Petri Net Approach, volume 16. Springer science & business media, 2010. URL: https://doi.org/10.1007/978-1-84996-474-6.
- [11] Kurt Lautenbach. Linear algebraic techniques for place/transition nets. In Petri Nets: Central Models and Their Properties: Advances in Petri Nets 1986, Part I Proceedings of an Advanced Course Bad Honnef, 8.–19. September 1986, pages 142–167. Springer, 1987.

- [12] A. J. Lawson, J. Swienty-Busch, T. Géoui, and D. Evans. The Making of Reaxys—Towards Unobstructed Access to Relevant Chemistry Information. In *The Future of the History of Chemical Information*, pages 127–148. ACS Publications, 2014. URL: https://doi.org/10.1021/bk-2014-1164.ch008.
- [13] M. A. Marsan, G. Balbo, G. Conte, S. Donatelli, and G. Franceschinis. Modelling with Generalized Stochastic Petri Nets. ACM SIGMETRICS Performance Evaluation Review, 26(2):2, 1998.
- [14] Mogens Nielsen, Lutz Priese, and Vladimiro Sassone. Characterizing behavioural congruences for petri nets. In CONCUR'95: Concurrency Theory: 6th International Conference Philadelphia, PA, USA, August 21–24, 1995 Proceedings 6, pages 175–189. Springer, 1995.
- [15] J. L. Peterson. Petri Net Theory and the Modeling of Systems. Prentice Hall PTR, USA, 1981.
- [16] J.L. Reed, T.D. Vo, C.H. Schilling, and B.O. Palsson. An Expanded Genome-Scale Model of Escherichia Coli K-12 (ijr904 gsm/gpr). Genome Biol, 4, 2003. URL: https://doi.org/10.1186/gb-2003-4-9-r54.
- [17] Paweł Sobociński. Representations of petri net interactions. In CON-CUR 2010-Concurrency Theory: 21th International Conference, CONCUR 2010, Paris, France, August 31-September 3, 2010. Proceedings 21, pages 554–568. Springer, 2010.
- [18] J. J. Tyson and B. Novák. Functional Motifs in Biochemical Reaction Networks. Annual Review of Physical Chemistry, 61:219–240, 2010. URL: https://doi.org/10.1146/annurev.physchem.012809.103457.
- [19] J. Van Brakel. Substances: The Ontology of Chemistry. In Philosophy of Chemistry, pages 191–229. Elsevier, Amsterdam, 2012. URL: https: //doi.org/10.1016/B978-0-444-51675-6.50018-9.
- [20] D. J. Wilkinson. Stochastic Modelling for Systems Biology. Chapman and Hall/CRC, NY, 2018. URL: https://doi.org/10.1201/9781351000918.